Organic Chemistry 10.1 – Intro

IB Chemistry

Topic 10 – Organic

Resource:

Brown, Ford, HL Chem

10.1 Introduction - 4 hours

- 10.1.1 Describe the features of a homologous series. (2)
- 10.1.2 Predict and explain the trends in boiling points of members of a homologous series. (3)
- 10.1.3 Distinguish between empirical, molecular and structural formulas. (2)
- 10.1.4 Describe structural isomers as compounds with the same molecular formula but with different arrangements of atoms. (2)
- 10.1.5 Deduce structural formulas for the isomers of the non-cyclic alkanes up to C6. (3)
- 10.1.6 Apply IUPAC rules for naming the isomers of the non-cyclic alkanes up to C6. (2)
- 10.1.7 Deduce structural formulas for the isomers of the straight-chain alkenes up to C6. (3)

10.1 Introduction - 4 hours

- 10.1.8 Apply IUPAC rules for naming the isomers of the straight-chain alkenes up to C6. (2)
- 10.1.9 Deduce structural formulas for compounds containing up to six carbon atoms with one of the following functional groups: alcohol, aldehyde, ketone, carboxylic acid and halide. (3)
- 10.1.10 Apply IUPAC rules for naming compounds containing up to six carbon atoms with one of the following functional groups: alcohol, aldehyde, ketone, carboxylic acid and halide. (2)
- 10.1.11 Identify the following functional groups when present in structural formulas: amino (NH2), benzene ring ( ) and esters (RCOOR). (2)
- 10.1.12 Identify primary, secondary and tertiary carbon atoms in alcohols and halogenoalkanes. (2)
  - 10.1.13 Discuss the volatility and solubility in water of compounds containing the functional groups listed in 10.1.9. (3)

Types of Reactant

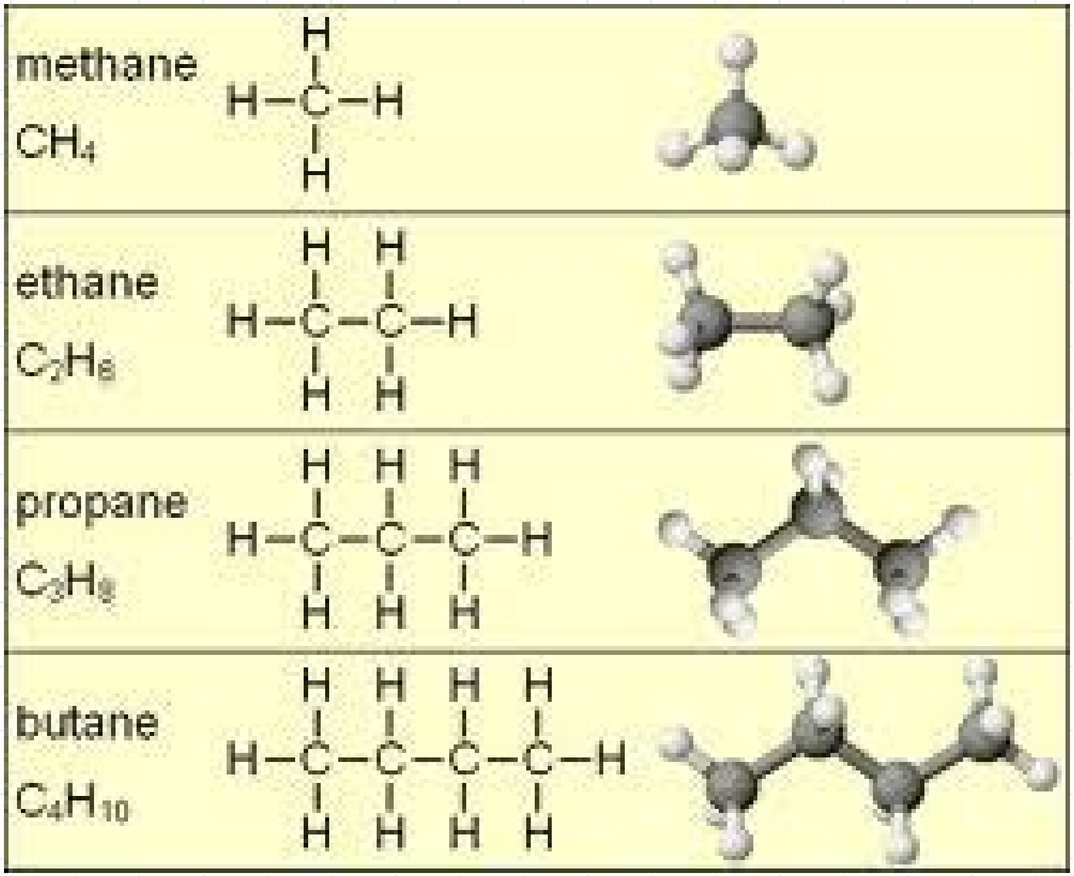
Saturated	Unsaturated
•Compounds which contain only single bonds •For example: alkanes	•Compounds which contain double or triple bonds •For example: alkenes, arenes
Aliphatics	**Arenes**
•Compounds which do not contain a benzene ring; may be saturated or unsaturated •For example: alkanes, alkenes	•Compounds which contain a benzene ring; they are all unsaturated compounds •For example: benzene, phenol
Electrophile (electron-seeking)	**Nucleophile (nucleus-seeking)**
•An electron-deficient species which is therefor attracted to parts of the molecules which are electron rich •Electrophiles are positive ions or have a partial positive charge •For example: NO_2^+ , H^+ , $Br^{\delta+}$	•An electron-rich species which is therefore attracted to parts of molecules which are electron deficient •Nucleophiles have a lone pair of electrons and may also have a negative charge •For example: Cl^- , OH^- , NH_3

10.1.1 Describe the features of a homologous series. (2)

- Differ by a CH_2
- Can be represented by the same general formula
- Show gradation in physical properties
- Have similar chemical properties

Members of Homologous Series…

… differ by a $–CH_2$ group



Members of Homologous Series…

… can be represented by the same general formula

Formula	Name
CH_4OH	Methan-1-ol
C_2H_5OH	Ethan-1-ol
C_3H_7OH	Propan-1-ol
C_4H_9OH	Butan-1-ol
$C_5H_{11}OH$	Pentan-1-ol
$C_6H_{13}OH$	Hexan-1-ol
$C_7H_{15}OH$	Heptan-1-ol
$C_8H_{17}OH$	Octan-1-ol

Members of Homologous Series…

… show gradation in physical properties

Alkane	Boiling Point
Methane, CH_4	-164
Ethane, C_2H_6	-89
Propane, C_3H_8	-42
Butane, C_4H_{10}	-0.5
Pentane, C_5H_{12}	36
Hexane, C_6H_{14}	69
Heptane, C_7H_{16}	98
Octane, C_8H_{18}	125

- Since the series differ by one $–CH_2$ they have successively longer carbon chains
  - Results in gradual trend of phy. Props
  - Not always a linear growth
  - Density and viscosity are other examples

Members of Homologous Series…

… show similar chemical properties

- As the have the same functional group
  - Ex.1 – the alcohols have a functional –OH group, which can be oxidized to form organic acids
  - Ex. 2 – the –COOH functional group, present in the homologous series of the **carboxylic acids**, is responsible for the acidic properties of these compounds

10.1.2 Predict and explain the trends in boiling points of members of a homologous series. (3)

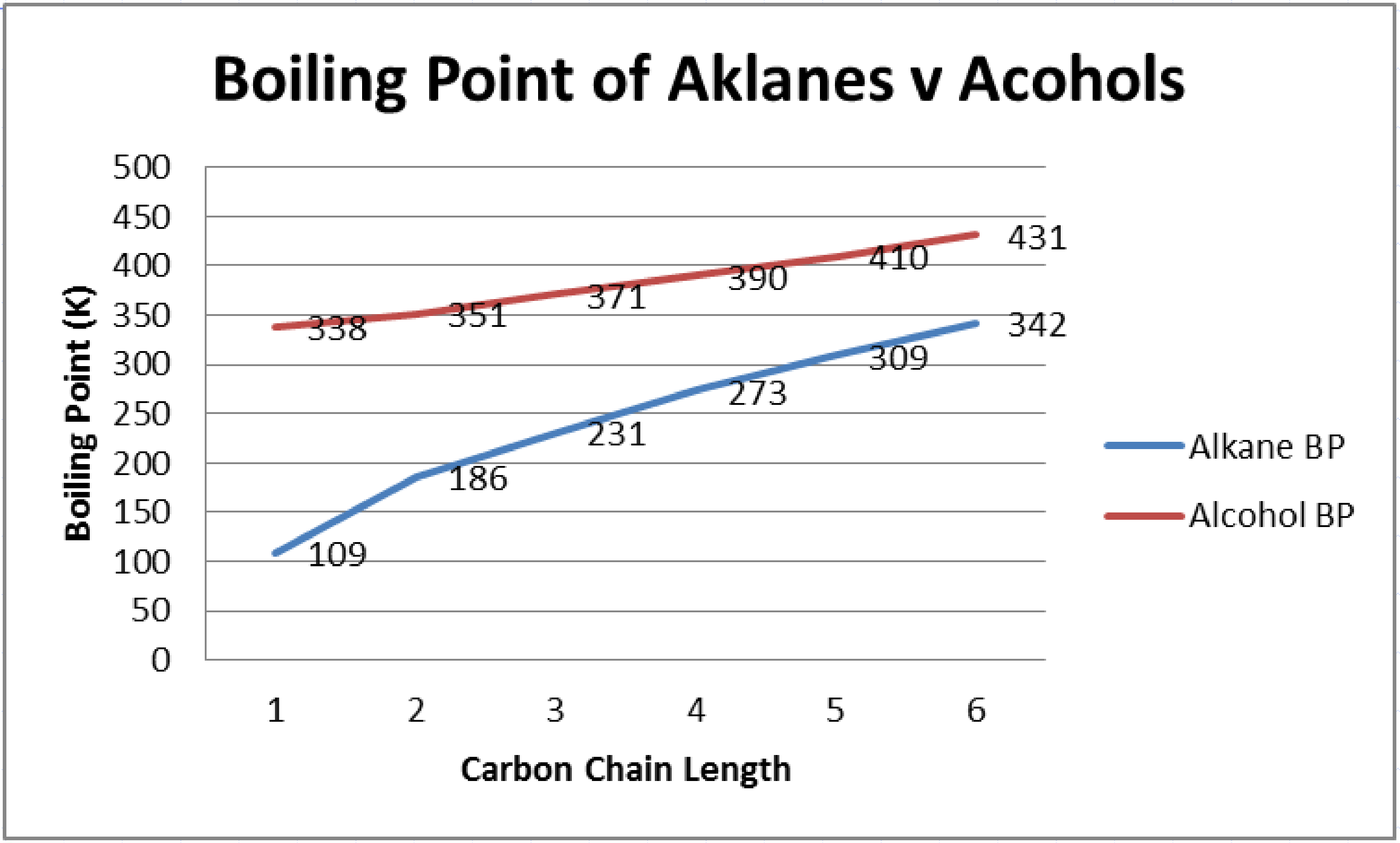
Alkane	Molecular Formula C_nH_{2n+2}	C atoms	M.P. (K)	B.P. (K)	B.P. Increasing	State at STP
Methane	CH_4	1	91	109		Gas
Ethane	C_2H_6	2	90	186		Gas
Propane	C_3H_8	3	83	231		Gas
Butane	C_4H_{10}	4	135	273		Gas
Pentane	C_5H_{12}	5	144	309		Liquid
Hexane	C_6H_{14}	6	178	342		Liquid

Because of increased van der Waals forces!

B.P. of Alcohols

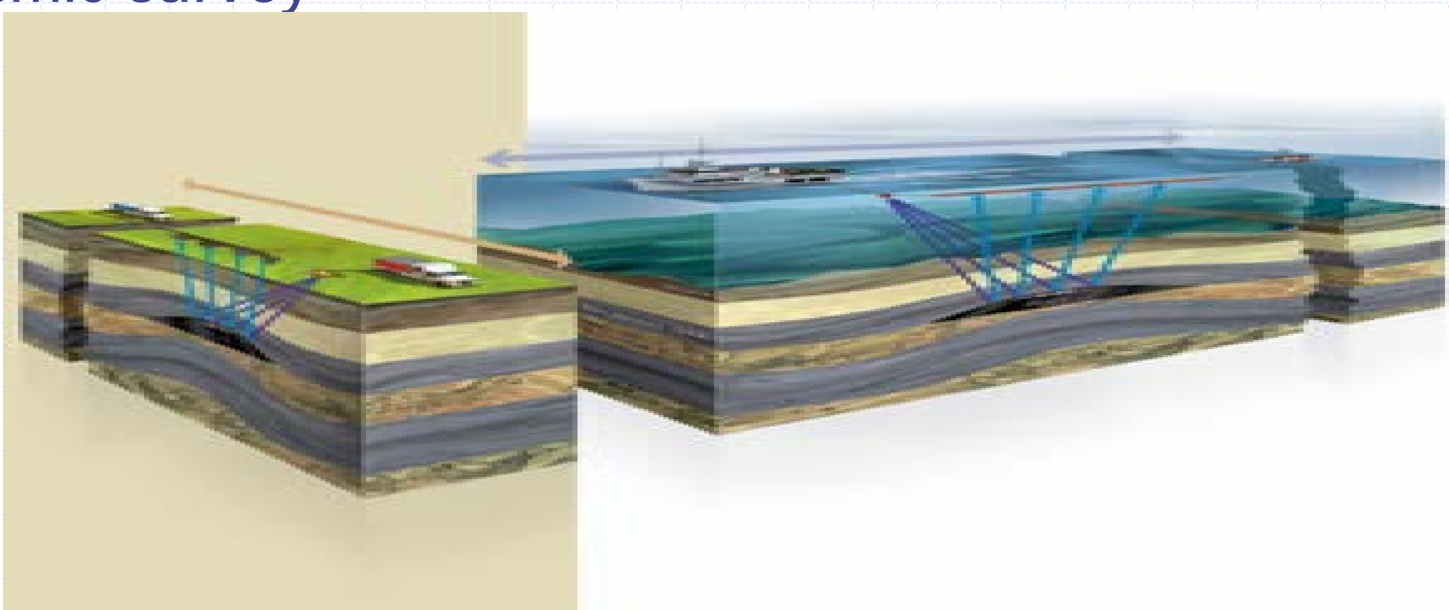
Alcohol	Molecular Formula $C_nH_{2n+2}O$ ($C_nH_{2n+1}OH$)	B.P. (K) @ STP	B.P. Increasing
Methanol	CH_4O (CH_3OH)	338	
Ethanol	C_2H_6O (C_2H_5OH)	351	
Propan-1-ol	C_3H_8O (C_3H_7OH)	371	
Butan-1-ol	$C_4H_{10}O$ (C_4H_9OH)	390	
Pentan-1-ol	$C_5H_{12}O$ ($C_5H_{11}OH$)	410	
Hexan-1-ol	$C_6H_{14}O$ ($C_6H_{13}OH$)	431	

Graph of BP trend



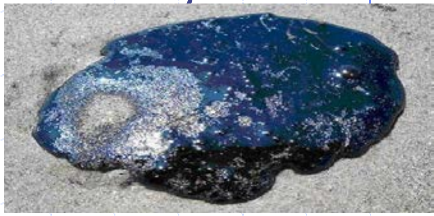
Finding Oil

- Crude oil today was made from mainly plankton that died about 150 million years ago. Their bodies did not decay normally due to lack of oxygen and with high pressures and temperatures, formed oil and natural gas.
- We can find oil by surveying the land and its topography
  - Look for dome shaped layers (cap rock or anti-cline)
  - Seismic survey



Distilling Crude Oil

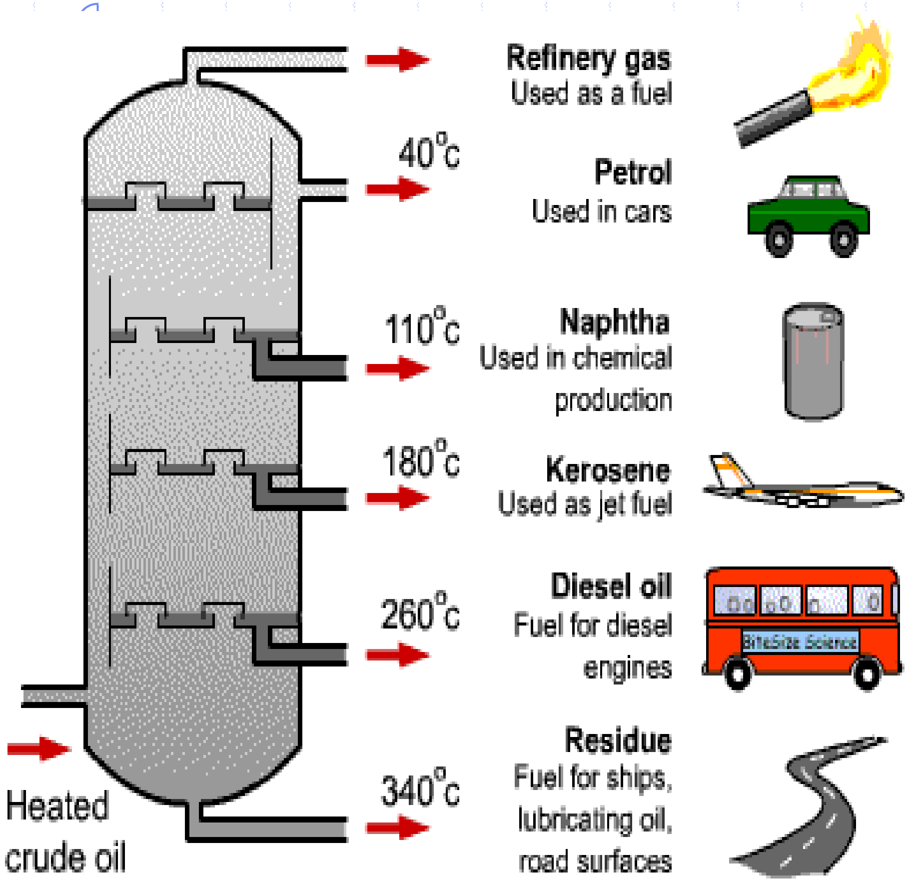
- When crude oil reaches the refinery it's a thick, black, and smelly liquid
  - This liquid contains long hydrocarbon chains



- At the refinery the long chains can be sorted out into groups of useful substances called **fractions**
  - We can separate these substances by **fractional distillation** which separates substances based on their boiling point

Fraction	Length	Color	Thickness	Reactivity
Low BP (up to 80C)	Short	Clear	Runny	Easily lit (flammable, clean flame)
Medium BP (80-150C)	Medium	Yellow	Thicker	Harder to light, some smoke
High BP (above 150C)	Long	Dark orange	Thick	Difficult to light, smoky flame

Fractional Distillation in Industry



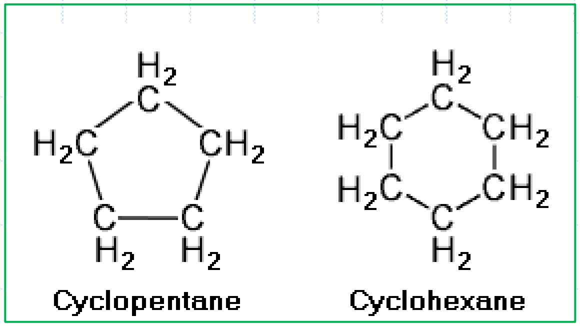
Fraction	Length of Carbon Chain
Petroleum gas	C_1-C_4
Petrol	C_4-C_{12}
Kerosine	C_{11}-C_{15}
Diesel	C_{15}-C_{19}
Lubricating Oil	C_{20}-C_{30}
Fuel Oil	C_{30}-C_{40}
Bitumen	C_{50} +

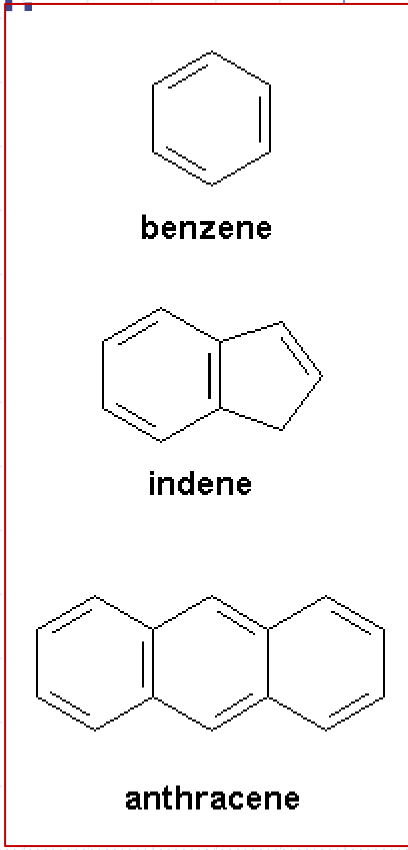
10.1.3 Distinguish between empirical, molecular and structural formulas. (2)

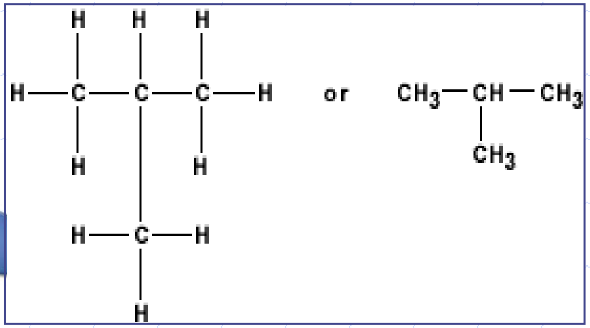
- Empirical formula
  - Simplest whole number ratio
  - Ethane CH_3
- Molecular formula
  - Actual number of atoms
  - Ethane C_2H_6
- Structural Formula
  - Full, condensed, stick, steriochemical

Hydrocarbons

- Hydrocarbons are organic compounds that are made up of only carbon and hydrogen.
- There are several different categories of hydrocarbons including:
  - Alkanes
  - Alkenes
  - Alkynes
  - Cyclic Hydrocarbons
  - Aromatic hydrocarbons
  - Branched chains







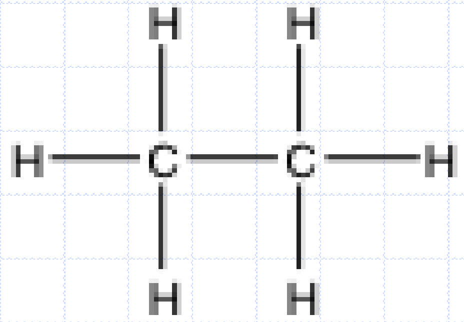
Double bonds with resonance (delocalization)

Empirical v Molecular Formulas

- The simplest whole number ratio of the atoms it contains. This formula can be derived from percentage composition data (from combustion analysis or mass spec). It is, however, of rather limited use on it's own, as it does not tell us the actual number of atoms in the molecule.
- Actual number of atoms of each element present. For example, the molecular formula of ethane is C_2H_6. It is therefore a multiple of the empirical formula, and so can be deduced if we know both the empirical formula and the relative molecular mass M_r.

Full Structural Formula

- Graphic formula or displayed formula – shows every bonded atom. Usually 90^o and 180^o angles are used to show the bonds because this is the clearest 2-D representation, although it is not the true geometry of the molecule



ethane

Condensed Structural Formula

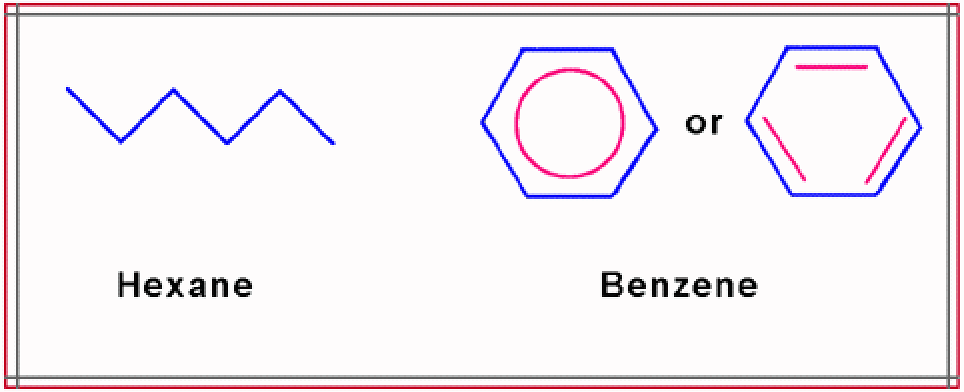
- Often omits bonds where they can be assumed, and groups atoms together. It contains the minimum information needed to describe the molecule non-ambiguously – in other words there is only one possible structure that could be described by its formula.

$$CH_3{-}CH_2{-}CH_2{-}CH_3$$

$$CH_3CH_2CH_2CH_3$$

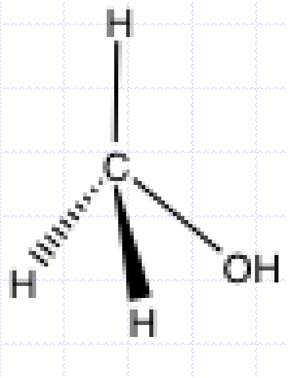
Stick model

- IB does not represent organic compounds using the stick model, but will accept your drawings as such.
- It is assumed that any intersection contains a carbon atom with the maximum number of hydrogen's attached (considering availability of bonds to C – total of 4 bonds)



Stereochemical Formula

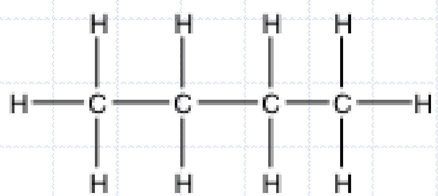
- Attempts to show the relative positions of atoms and groups around carbon in three dimensions. The convention is that a bond sticking forwards from the page is shown as a solid, enlarged wedge, whereas a bond sticking behind the page is shown as a dotted line. A bond in the plane of the paper is a solid line.



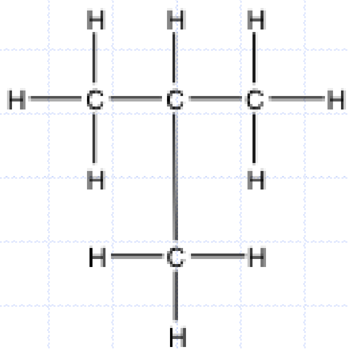
methanol

10.1.4 Describe structural isomers as compounds with the same molecular formula but with different arrangements of atoms. (2)
10.1.5 Deduce structural formulas for the isomers of the non-cyclic alkanes up to C6. (3)

- Different arrangements of the same atoms make different molecules
- Molecular formula shows the atoms that are present in a molecule, but gives no information on how they are arranged. Consider, for example, C_4H_{10}
- Each isomer is a distinct compound, having unique physical and chemical properties.



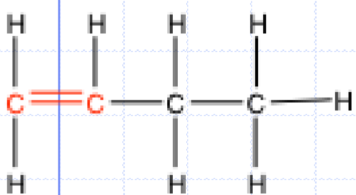
butane
boiling point -0.5°c



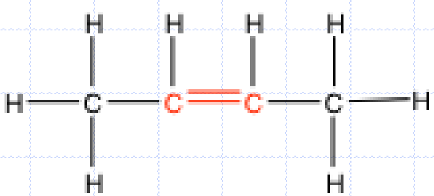
2-methyl propane
boiling point -11.7°c

Structural Isomers of Alkenes

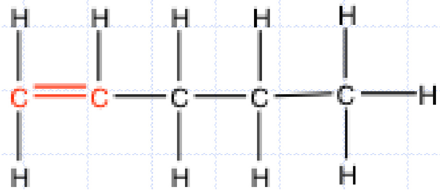
10.1.7 Deduce structural formulas for the isomers of the straight-chain alkenes up to C6. (3)



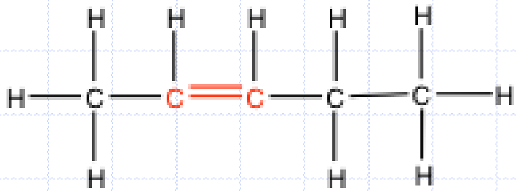
but-1-ene



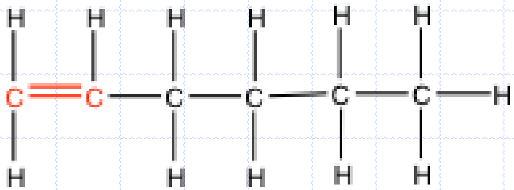
but-2-ene



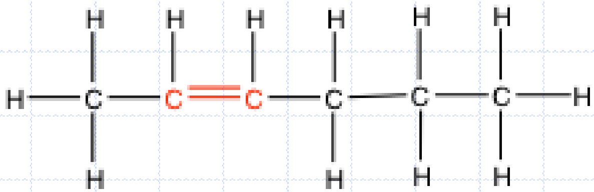
pent-1-ene



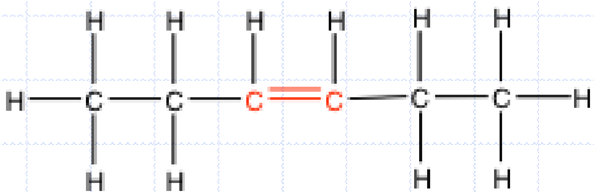
pent-2-ene



hex-1-ene



hex-2-ene



hex-3-ene

IUPAC

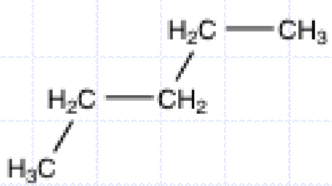
- Nomenclature for Organic Compounds: the IUPAC system
  - International Union of Pure and Applied Chemistry
  - Rule 1: Identify the longest straight chain of carbons
  - Rule 2: Identify the functional group
  - Rule 3: Identify the side chains or substituent groups

IUPAC Rule 1: Longest Chain

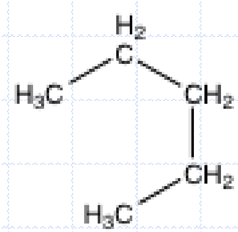
10.1.6 Apply IUPAC rules for naming the isomers of the non-cyclic alkanes up to C6. (2)

# C atoms in longest	Stem in IUPAC name	Example
1	meth-	CH_4 methane
2	eth-	C_2H_6 ethane
3	prop-	C_3H_8 propane
4	but-	C_4H_{10} butane
5	pent-	C_5H_{12} pentane
6	hex-	C_6H_{14} hexane

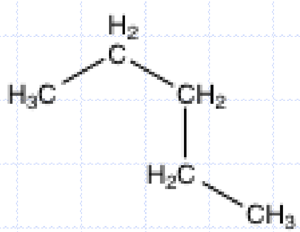
Note: ‘straight chain’ does not mean just 180º angles or unbranched chains of carbon atoms. Be careful, do not be confused by the way the molecule may appear on paper because of free rotation around the carbon-carbon single bonds. Example, all three below are the same….



pentane



pentane



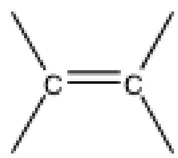
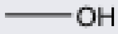
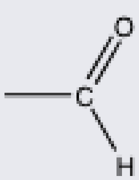
pentane

IUPAC Rule 2: Functional Group

- The functional group is described by a specific ending (or suffix) to the name, that replaces the –ane ending of the name of the parent alkane. The suffixes used for some common functional groups are in the slides to follow. Those marked * will have slides with further information.

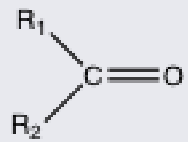
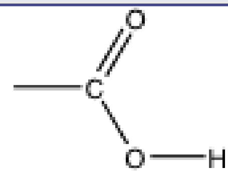
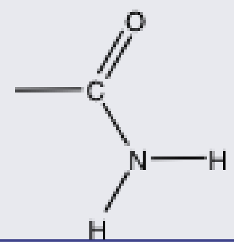
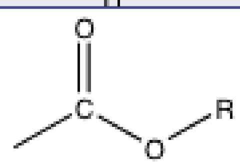
Functional Groups

10.1.9 Deduce structural formulas for compounds containing up to six carbon atoms with one of the following functional groups: alcohol, aldehyde, ketone, carboxylic acid and halide. (3)

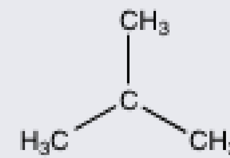
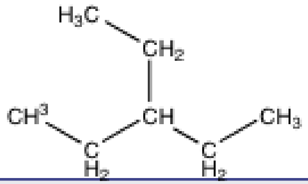
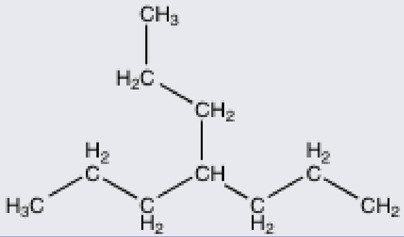
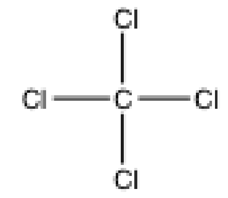
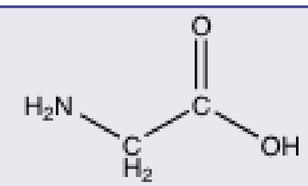
Name	**Functional Group**	**Suffix in IUPAC name**	**Example of compound**
Alkane		-ane	C_3H_8 propane
Alkene		-ene	$CH_3CH{=}CH_2$ propene
Alcohol		-anol	C_3H_7OH propanol
Amine*		-anamine	$C_3H_7NH_2$ propanamine
Aldehyde		-anal	C_2H_5CHO

Functional Groups

10.1.10 Apply IUPAC rules for naming compounds containing up to six carbon atoms with one of the following functional groups: alcohol, aldehyde, ketone, carboxylic acid and halide. (2)

Name	Functional Group	Suffix	Example
Ketone		-anone	CH_3COCH_3 propanone
Carboxyllic acid		-anoic acid	C_2H_5COOH Propanoic acid
Amide*		-anamide	$C_2H_5CONH_2$ propanamide
Ester		-anoate	$C_2H_5CHOH_3$ methyl propanoate
Nitrile (HL)		-anenitrile	C_2H_5CN propanenitrile

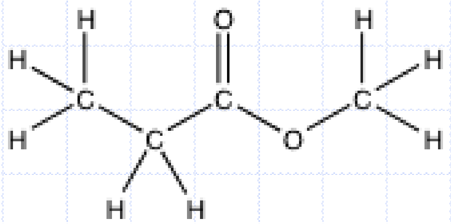
IUPAC Rule 3: Side Chains

Side Chain	Prefix in IUPAC	Example of Compound
$-CH_3$	methyl-	$CH_3CH(CH_3)CH_3$ 2-methylpropane 
$-C_2H_5$	ethyl-	$CH(C_2H_5)_3$ 3-ethylpentane 
$-C_3H_7$	propyl-	$CH(C_3H_7)_3$ 4-propylheptane 
-F , -Cl , -Br , -I	fluoro- , chloro- , bromo- , iodo-	CCl_4 Tetrachloromethane 
$-NH_2$	amino-	$CH_2(NH_2)COOH$ 2-aminoethanoic acid 

Ester Functional Group

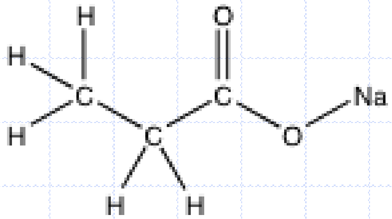
10.1.11 Identify the following functional groups when present in structural formulas: amino (NH2), benzene ring ( ) and esters (RCOOR). (2)

- Esters are organic salts where the alkyl group of the alcohol has replaced the hydrogen of the carboxylic acid. Their name puts the alkyl group first followed by the name of the acid anion, for example:



methyl propionate

$C_2H_5COOCH_3$



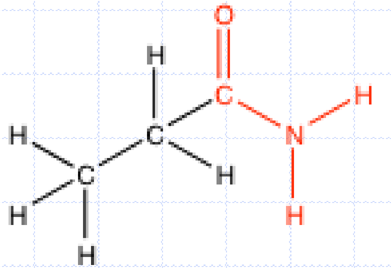
sodium propionate

C_2H_5COONa

Amide Functional Group

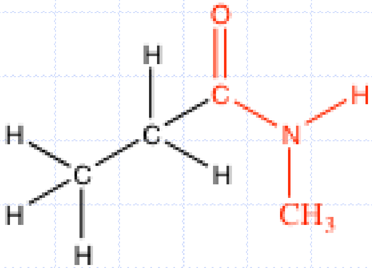
- Amides are acid derivatives where the –OH of the acid has been replaced by $–NX_2$. Primary amides have an $–NH_2$ group; secondary and tertiary amides are substituted with respectively one and two alkyl groups bonded to the nitrogen. In these cases the substituent groups are named using N- and N,N- before the substituent.

Primary amide..



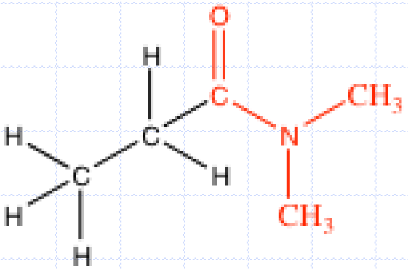
propionamide

Secondary amide..



N-methylpropionamide

Tertiary amide..

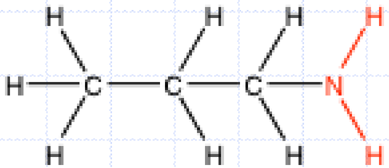


N,*N*-dimethylpropionamide

Amine Functional Group

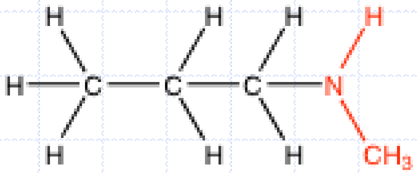
- Primary amines have an $–NH_2$ group which can undergo substitution by alkyl groups, giving rise to secondary and teriary amines. These are named in a similar way to the amides, using N- to show the position of the substituents

Primary amine..



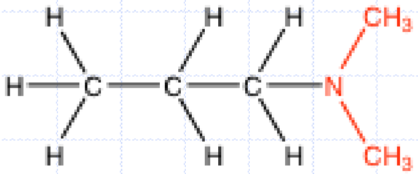
propan-1-amine

Secondary amine..



N-methylpropan-1-amine

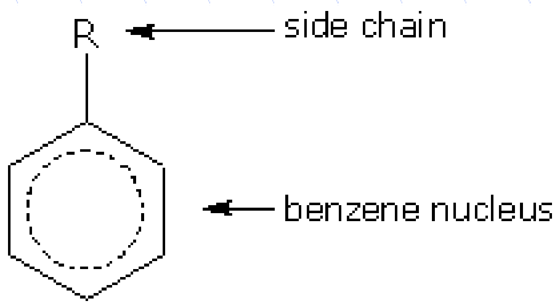
Tertiary amine..

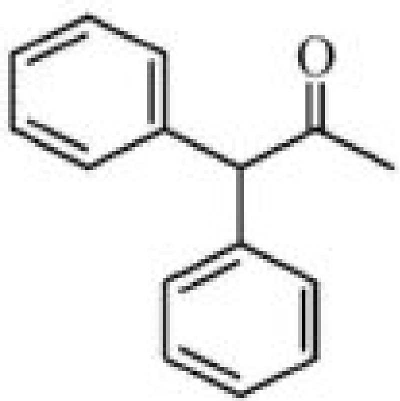


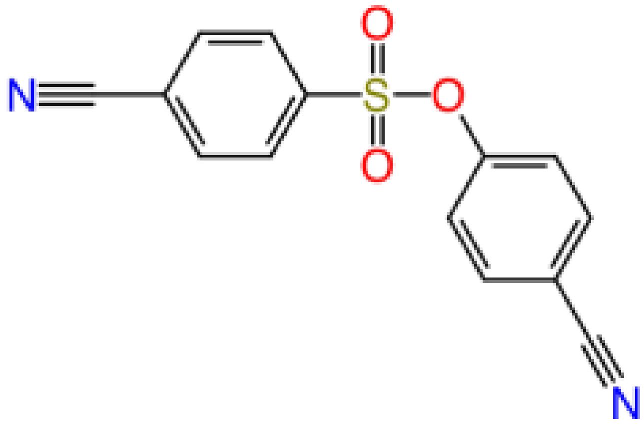
N,*N*-dimethylpropan-1-amine

Benzene Ring Addition

- The benzene ring itself is very flammable and is known to be colorless and a carcinogen
- It is often used in chemistry as a non-polar solvent as it's fairly volatile but can exist as a liquid given proper conditions.
- Consists of resonating pi (double) bonds
- It's an aromatic hydrocarbon

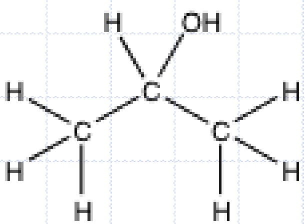




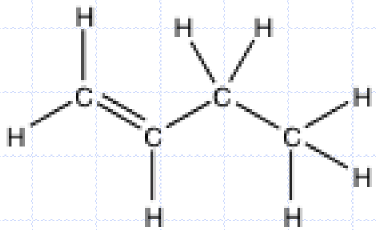


Position of Functional Group

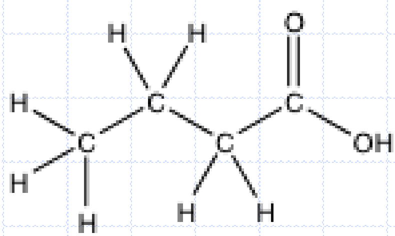
- Shown by a number between hyphens inserted before the functional group ending. The number refers to the carbon atom to which the functional group is attached when the chain is numbered starting at the end that will give the smallest number to the group.



propan-2-ol

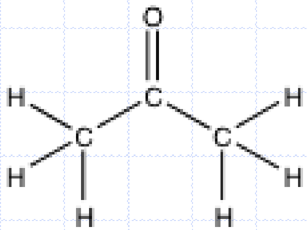


but-1-ene



butyric acid

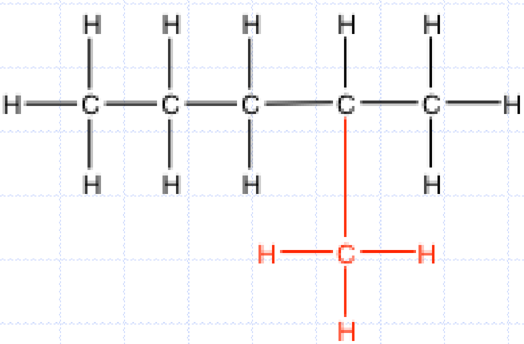
aka, butanoic acid



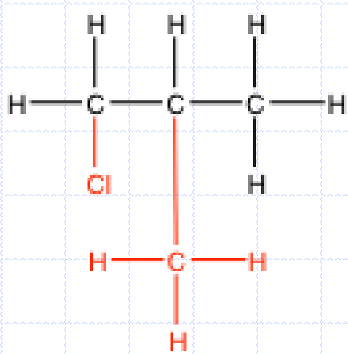
propan-2-one

When >1 functional group

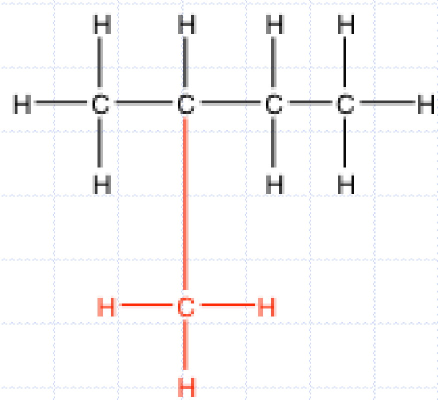
- Some suffix's may become prefix's
  - $-NH_2$ can be amino- prefix or –amine suffix
- If more than one of the same functional group we use prefixes di-, tri-, tetra- before the name



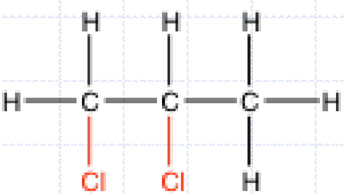
2-methylpentane



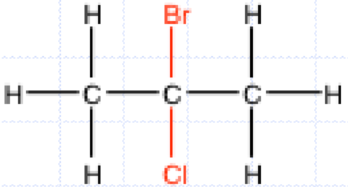
2-bromo-2-chloropropane



2-methylbutane



1,2-dichloropropane



1-chloro-2-methylpropane

(oops, switch the name)

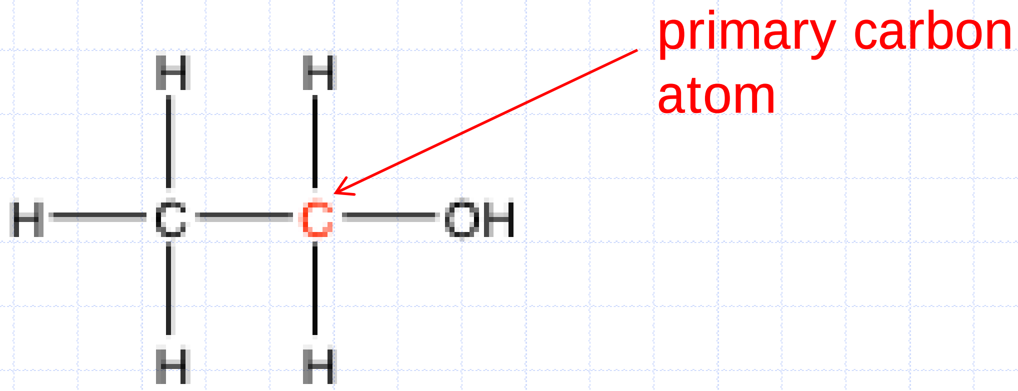
Classes of Compounds

10.1.12 Identify primary, secondary and tertiary carbon atoms in alcohols and halogenoalkanes. (2)

- The activity of a functional group is often influenced by its position in the carbon chain, identified as:
  - Primary carbon atom
  - Secondary carbon atom
  - Tertiary carbon atom

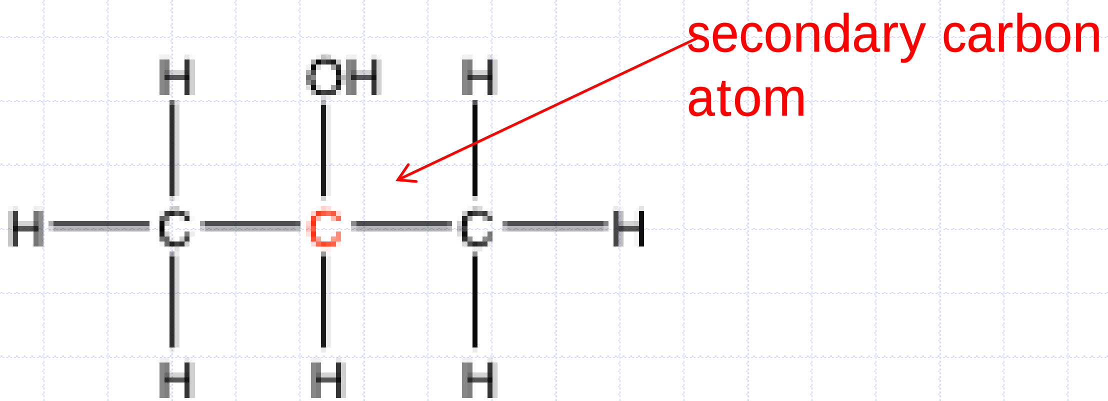
Primary Carbon Atom

- Is attached to the functional group and also to at least two hydrogen atoms. Molecules with this arrangement are known as primary molecules.
- For example, ethanol C_2H_5OH is a primary alcohol:



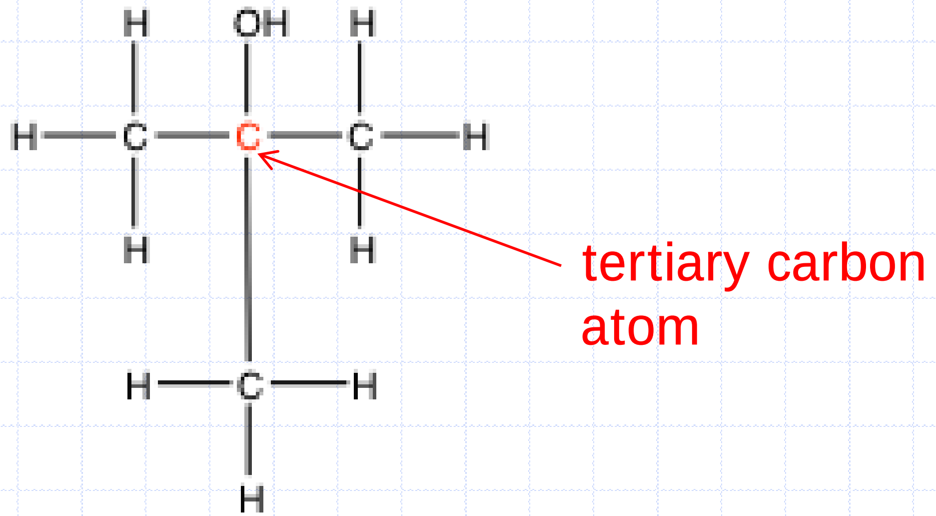
Secondary Carbon Atom

- Is attached to the functional group and also to one hydrogen atom and two alkyl groups. These molecules are known as secondary molecules
- For example, propan-2-ol, $CH_3CH(OH)CH_3$ is a secondary alcohol:



Tertiary Carbon Atom

- Is attached to the functional group and is also bonded to three alkyl groups and so has no hydrogen atoms. These molecules are known as tertiary molecules.
- For example, 2-methylpropan-2-ol, $C(CH_3)_3OH$ is a tertiary alcohol:



Trends in Physical Properties

10.1.13 Discuss the volatility and solubility in water of compounds containing the functional groups listed in 10.1.9. (3)

- We have seen that the structure of organic compounds can be thought of in terms of two parts
  - A framework consisting of carbon and hydrogen only, known as the **hydrocarbon skeleton**. This differs in size in different members of the same homologous series.
  - A functional group. This differs in identity in different homologous series.
- Both of these components influence the physical properties of a compound and must each be considered when comparing properties such as volatility and solubility in water

Volatility of Organics

- Volatility: a measure of how easily a substance changes into the gaseous state – highly volatile means the compound has a low boiling point.

Hydrocarbon Length effect on Volatility

- Higher members have larger molecules and stronger van der Waals' forces between them.
- Boiling Point increases ⇧.
- Lower members gases (g) or liquids (l)
- Higher likely solids (s)
- Branched chain isomers have lower boiling points (and intermolecular attractions) than straight-chain isomers.

Functional Group effect on Volatility

- Polar groups develop dipole-dipole interactions with neighboring molecules which raise the boiling point.
- For example:
  - Ethanol C_2H_5OH $M_r=46$ BP=78^{o}c
  - Propane C_3H_8 $M_r=44$ BP=-42^{o}c

The effect on volatility of the different functional groups as follows:
Most Volatile Least Volatile alkane > halogenalkane > aldehyde > ketone > alcohol > carboxylic acid
van der Waals' → dipole-dipole interaction → hydrogen bonding Increasing strength of molecular interaction → Increasing boiling point →

Solubility in Water

- Solubility is largely determined by the extent to which the solute molecules are able to interact and form hydrogen bonds with water. Depends once again on:
  - Hydrocarbon skeleton
  - Functional Group

Hydrocarbon Chain Effect on Solubility

- As this part of the molecule is non-polar and unable to form hydrogen bonds with water, it does not contribute to the solubility of the molecules. Therefore, higher members of all homologous series are less soluble than lower members

Functional Group effect on Solubility

- Molecules with functional groups that enable hydrogen bonds to form with water include **alcohols**, the **carboxylic acids** , and the **amines**. Aldehydes, ketones, amides and esters are less soluble, while halogenalkanes, alkanes and alkenes are insoluble.